

On a recent very simple generalization of DMT theory of adhesion

M.Ciavarella
 Politecnico di BARI.
 V.le Gentile 182, 70125 Bari-Italy.
 Email mciava@poliba.it

February 11, 2016

Abstract

As the interest in adhesion is shifting towards smaller and smaller scales, the well known Tabor adhesion parameter decreases and the DMT theory is frequently considered to be the appropriate limit. A very attractive much simplified version of DMT has been proposed in a recent investigation of rough contacts by Pastewka & Robbins (PNAS, 111(9), 3298-3303, 2014) which seems to work in very general conditions in numerical experiments. However, when comparing this calculation to the known theories for the sphere, surprisingly large conflicts occur, and the reason for the success of the numerical experiments is obscure.

Keywords: Adhesion, Greenwood-Williamson's theory, rough surfaces

1 Introduction

Pastewka & Robbins (2014, PR in the following) have made a quite interesting generalization of the DMT theory in their numerical simulations involving atomistics rough solids. They postulate that the attractive forces have little effect on the detailed morphology of the repulsive contact area, the repulsive force and mean pressure are also nearly unchanged, so that they are close to the Derjaguin-Muller-Toporov (DMT) limit (Derjaguin et al., 1975, Muller et al., 1980, 1983). They then notice that in the "attractive" regions of area A_{att} , the pressure is simply the theoretical strength of the material, $\sigma_{th} = w/\Delta r$, where w is surface energy, and Δr is a range of attraction. This leads them to suggest a very simple model for adhesion, by considering the first order expansion of the separation distance between two contacting bodies under repulsive forces only, which scales as distance^{3/2} virtually for any geometry, and equating the peak separation to the characteristic distance Δr , they find the size of the attractive regions. The special behaviour of rough contact leads to a very simple picture

in which characteristic sizes of repulsive and attractive regions are defined by two almost constant length scales for any given system, d_{rep} and d_{att} (their size is said to vary less than 25% varying the load) so that $A_{rep} = Pd_{rep}/\pi$ and $A_{att} = Pd_{att}$, where a perimeter P increases with load. The model is so simple that it permits them to extrapolate criteria for "stickiness" in very general terms, and it is worth comparing it with the classical DMT theory, to see the order of approximation involved in the very simple calculation, in an instructive case.

In fact, there has been so much discussion in the literature about the DMT theory (see next paragraph), that it is surprising that PR propose such a back-of-the-envelope calculation without encountering any significant error.

2 The DMT theories

It is often believed that DMT is the limit for Tabor parameter

$$\mu = \left(\frac{Rw^2}{E^{*2}\Delta r^3} \right)^{1/3} = \left(\frac{Rl_a^2}{\Delta r^3} \right)^{1/3} \rightarrow 0 \quad (1)$$

where R is the radius of the sphere, w is surface energy and E^* plane strain modulus of the material ($l_a = w/E^*$ is an alternative way to measure adhesion as a length scale).

Greenwood (2007) has clearly demonstrated that this typical statement is "*completely unwarranted: the Tabor parameter governs the transition from rigid body behaviour to JKR behaviour*". The reason is that the assumptions in DMT theory make the predictions consistently worse than assuming the sphere to be rigid, and indeed Greenwood proceeds to suggest a "semi-rigid" theory of adhesion, in which the sphere is first assumed rigid, the surface forces are estimated from the undeformed shape, and with these surface forces, the displacement on the axis of the sphere is computed.

The story of these theories starts with Bradley (1932) who obtained the adhesive force between two rigid spheres, equal to $2\pi R w$, and Derjaguin (1934) who reobtained this results in a simpler way with the so called *Derjaguin approximation* (the force between elements of curved, inclined surfaces is the same as that between elements of plane, parallel surfaces), and finally that the attractive force between spheres separated by a gap h_0 is insensitive to the exact shape of the force between two plane surfaces at distance h , i.e. $\sigma(h)$, as it can be computed from

$$P = 2\pi R \int_{h_0}^{\infty} \sigma(h) dh \quad (2)$$

However, Derjaguin (1934) in the case of elastic spheres found 1/2 the pull-off force. JKR (Johnson Kendall and Roberts 1971) developed their different theory assuming adhesive forces occur entirely within the contact area, obtaining 3/4 of the Bradley pull-off value, and hence the factor seemed to cause a conflict. Derjaguin then developed with his colleagues the DMT theory (Derjaguin *et al.*,

1975) which is a "thermodynamic method" which caused few troubles. Indeed, DMT leads to Bradley result for the force, but the attraction forces outside the contact add a contribution ("overload", according to Maugis (2000) denomination) which decreases from $2\pi R w$ to $\pi R w$ when the approach increases, which was shown to be an error intrinsic in the "thermodynamic method" by Pashley (1984). Indeed, Pashley (1984) showed that the force between a *truncated rigid* sphere and a flat is constant and is given by $2\pi R w$ independent on the contact radius. Since the Hertzian profile is for any contact radius size, closer to the flat surface than the rigid spherical profile, the force should become larger than $2\pi R w$ as the area of contact increases. He then integrated the full Lennard-Jones potential as

$$P = 2\pi \frac{8w}{3a_0} \int_a^\infty \left[\left(\frac{a_0}{h} \right)^3 - \left(\frac{a_0}{h} \right)^9 \right] r dr \quad (3)$$

where for the Hertzian profile at a given value of contact area a

$$h(\varepsilon, a, r) = \varepsilon + \frac{1}{\pi R} \left[a \sqrt{r^2 - a^2} - \sqrt{2a^2 - r^2} \arctan \sqrt{\frac{r^2}{a^2} - 1} \right] \quad (4)$$

where ε is added as there is some equilibrium distance when considering repulsive forces. Pashley then obtained that the overload in fact increases with a/R , being about double, $4\pi R w$, as $a/R = 0.1$ (which is clearly already quite high deformation for an elastic theory). Muller, Derjaguin and Toporov (MDT, 1983) revisiting the DMT theory, used a full Lennard-Jones potential as had been used in an earlier full numerical analysis (MYD, Muller et al., 1980), but again using the 'thermodynamic' method as in the original DMT paper: pull-off is found when the contact area is zero only for $\mu < 0.24$, but for $\mu > 0.24$ the overload increases with approach so that the pull-off force exceeds the Bradley value for small positive value of the approach.

Finally, Maugis (1991, 2000) revisited the DMT theory, and suggested the overload should not depend on approach and indeed be constant, given by the pull-off load, $2\pi R w$. This is not what Pashley (1984) obtains with the force method even in the most refined form using the full L-J potential. As we are in fact examining the generalization of DMT theory with the force method suggested by PR, it is important to see the consequences. Greenwood (2007) indeed suggests Maugis' version of DMT is merely an approximation, referred to as DMT-M, and it is the most frequently quoted as DMT's contribution. However, since Maugis (1991, 2000) clearly shows that DMT-M is obtained in the limit of his Dugdale model when the Tabor parameter decreases to 0, it is clear that DMT-M remains the best approximation, as the force method and the DMT approximation has some subtle problems. Greenwood (2007) clarifies that for small values of the approach, the force evaluation needs care, as we need integrating the difference between the surface forces for the gap with a rigid sphere and those for the Hertzian gap, finds the DMT model to be constantly worse than assuming the sphere to be rigid, but does not discuss the issue of

overload further: should a better approximation remain that of the *truncated rigid* sphere and hence a constant overload?

Maugis suggests another problem in DMT theory: that continuity of stresses is not possible if we move from the Hertzian pressure distribution, which is zero at the edge where gap is just the equilibrium distance ε , to a positive value of tension just outside: the problem doesn't arise with L-J potential of course. He suggests the DMT limit is seen only when the region outside the contact is strictly infinitely large, although the integral remains finite, to $2\pi R w$. More likely, Maugis in fact obtains the DMT limit as the limit of his Dugdale model, rather than by integration of the forces in the DMT sense, as otherwise he would have incurred in the troubles described in details by Greenwood (2007).

When making further approximations in the force method, the results cannot certainly improve.

3 PR - DMT model

Returning therefore to the PR model, the simple estimate they suggest would work extremely well for a rigid sphere. In fact, the shape of the separation function is simply $h(x) = x^2/(2R)$ as there is no deformation, and imposing the separation is equal to Δr gives¹ $x_{att}^2 = 2R\Delta r$. If we then assume the mean pressure in the attractive region is simply $w/\Delta r$, the force $N = \frac{w}{\Delta r}\pi x_{att}^2 = \frac{w}{\Delta r}\pi 2R\Delta r = 2\pi R w$ the well known Bradley result, independent on the estimate of Δr in fact.

However, as we consider the case with some actual compression, the situation is obviously more problematic. They suggest to use the first order term in the asymptotic expansion of the separation function, which is universally given by the same function for simple geometries like spheres, cones, or cylinders. Indeed, the only length scale that enters is the radius of the contact area. As the contacting region in their numerical simulations resembles one with a 2D contact with constant average diameter d_{rep} , they use the standard prefactor for a cylinder and hence use

$$2\frac{h(x)}{d_{rep}} = \frac{\sqrt{8}}{3}h'\left(\frac{2x}{d_{rep}}\right)^{3/2} \quad (5)$$

where h' is the slope at the contact edge, which in their theory they estimate from a random process. In order to compare with some known results, we shall make the comparison of this procedure in the case of a sphere, where $h' = d_{rep}/(2R)$. The first order expansion of (4), $h \simeq \frac{\sqrt{2a}}{R}\frac{8}{3\pi}x^{3/2}$, differs indeed only by the prefactor $\frac{8}{3\pi} = 0.85$ being a little larger than PR equation (5) considering $a = d_{rep}/2$, which gives a prefactor $\frac{2}{3}$ (we have omitted the constant term a_0 which in a DMT model with no repulsive force should not be included). We shall maintain the prefactor in the original PR equation, as they

¹We avoid the notation d_{att} as d_{att} will have to do with an annulus shape, whereas x_{att} here is a radius of a circular region.

suggest it is more useful for rough surface typical asperity contacts. PR discuss that Δr can be estimated for arbitrary potential, but is of the order of a_0 , or a little smaller. With the 9-3 Lennard-Jones potential $\Delta r = 1.15a_0$, while for 12-6 LJ, $\Delta r = 0.62a_0$. If we equate this separation law with the range of attractive forces, Δr , we obtain the lateral distance defining the size of attractive region (which is a circular annulus of size d_{att})

$$d_{att} = \left[\frac{\left(\frac{3}{2}R\Delta r\right)^2}{d_{rep}} \right]^{1/3} \quad (6)$$

It is clear that this equation, having been obtained with a first order expansion in $h(x)$, is valid if $d_{att} \ll d_{rep}$, and this introduces obviously a strong limitation when the contact radius is small, and also a maximum radius of the sphere for any given d_{rep} : for $d_{rep} = 2\Delta r = 2a_0$, we need $\frac{R}{a_0} < 2.66$; for $d_{rep} = 200a_0$, then $\frac{R}{a_0} < 26500$. For large contact or large compression, a stricter limit on radius comes from the range of small Tabor parameters. For example, for $l_a/a_0 = 0.05$ of the LJ potential, the assumption $\mu < 1$ in (1) implies $\left(\frac{R}{a_0}\right) < 400$.

If we now consider the spherical case, following exactly the steps in PR theory, the attractive load is

$$P_{att} = \pi d_{rep} d_{att} \frac{w}{\Delta r} = \pi d_{rep} \frac{w}{\Delta r} \left[\frac{\left(\frac{3}{2}R\Delta r\right)^2}{d_{rep}} \right]^{1/3} = 3^{2/3} \pi w R \left(\frac{\delta}{\Delta r} \right)^{1/3} \quad (7)$$

where δ is the compression (or approach) of the sphere, given by Hertz theory as $\delta = d_{rep}/(2R)$. This model is different from the DMT-M model for a sphere with constant overload. The simplifications we have adopted in the analysis are evident at small compressions, as there is no adhesive force for zero compression, unlike all the DMT theories (which of course consider a better integration of the force) and pull-off of the classical DMT theory is obtained only (unrealistically) for positive compression

$$\frac{\delta^*}{\Delta r} = \frac{8}{9}$$

Above this point, with further compression, the adhesive overload continues to increase, but this is not due to the approximation of taking the first order in the separation function. For example, for $d_{rep} = 200a_0$, assuming the $\mu = 1$ case $R = 400a_0$,

$$P_{att} = 2\pi w R \frac{3^{2/3}}{2} \left(\frac{200^2}{4 * 400} \right)^{1/3} = 2\pi w R \times 3.04 \quad (8)$$

and increase of a factor 3. Notice that in this case $\frac{d_{rep}/2}{R} = \frac{100}{400} = 0.25$ and hence extrapolating the results of Fig.3 in Pashley (1984) obtained with the full 3-9 L-J potential and the full expression of Hertzian separation function, this result seems extremely similar: this is another source of error, intrinsic in the force method.

4 Dimensionless notation

We can illustrate the PR theory for the sphere more conveniently with dimensionless notation using Tabor parameter

$$\hat{\delta} = \delta / (\mu \Delta r) \quad ; \quad \hat{P} = P / (\pi R w) \quad (9)$$

and (7) becomes

$$\hat{P}_{att} = 3^{2/3} \left(\hat{\delta} \mu \right)^{1/3} \quad (10)$$

The point where there is exact coincidence with DMT-M is now $\hat{\delta} = \left(\frac{2}{3^{2/3}} \right)^3 / \mu = 0.89/\mu$ which obviously increases without limit for low μ .

Adding the Hertzian contribution, and writing also DMT-M (constant overload), and the JKR theory (Johnson, et al., 1971)²

$$\hat{P}_{DMT-M} = \frac{4}{3\pi} \hat{\delta}^{3/2} - 2 \quad (11)$$

$$\hat{P}_{PR} = \frac{4}{3\pi} \hat{\delta}^{3/2} - 3^{2/3} \left(\hat{\delta} \mu \right)^{1/3} \quad (12)$$

$$\hat{P}_{JKR} = \hat{P}_0 - 1.1 \left(\hat{\delta} - \hat{\delta}_0 \right)^{1/2} + 0.43 \left(\hat{\delta} - \hat{\delta}_0 \right)^{3/2} \quad (13)$$

where $\hat{\delta}_0 = -\frac{3}{4}\pi^{2/3}$, $\hat{P}_0 = 5/6$ are the JKR values at pull-off in displacement control.

The plots are shown in Fig.1 for $\mu = 0.1, 0.5, 1$. The error for small approaches was expected, since the first order expansion of the separation gap tends to work less well there, and one should integrate carefully the forces. Another difference reducing the adhesion forces comes from the prefactor in the assumed form of separation, which reduces the size of attractive regions. However, reduction of adhesive forces does not come only for the prefactor, as it is clear from the equations above: the DMT-PR theory simply for Tabor parameter near zero leads to the Hertz theory $\left(\hat{\delta} \mu \right) = 0$, which is here not plotted for clarity of representation, as it is simply the DMT-M curve shifted up by a constant factor 2. Further, the overload increase becomes quite large for intermediate Tabor parameters, and conflicts with the most established form of DMT theory (that given by Maugis).

Hence, there is only a relatively narrow range of regimes where this approximated theory can give reasonable results.

²JKR is presented in a curve fitted form in order to be easily used.

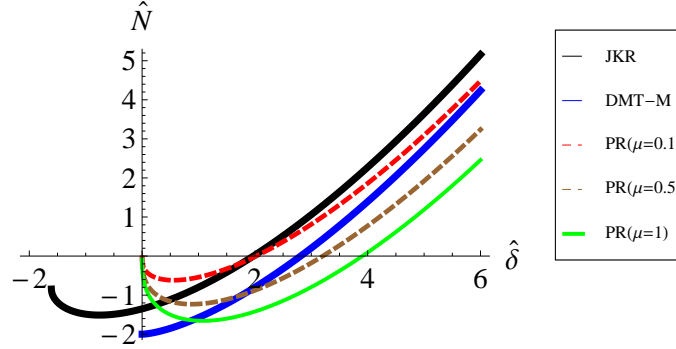


Fig.1. Curves load-approach for JKR, DMT-M, and DMT-PR theories, for the sphere. PR is plotted for Tabor parameter $\mu = 0.1, 0.5, 1$

5 Discussion

Given the extensive simulations in the PR paper, it is not clear how the PR version of the DMT model can work reasonably well over different conditions, including a realistic range of μ : PR simulations are said to be accurate for Maugis version of Tabor parameter $\lambda = \left(\frac{9}{2\pi}\right)^{1/3} \mu = 1.13\mu$ which exceeds unity (they do not say unfortunately what is the inferior limit). It is true that DMT theories (or "force methods", or perhaps Derjaguin–Pashley theories as Greenwood (2007) suggests) have not been discussed in details other than in the pull-off limit value, but the Maugis solution is clearly shown to tend to the DMT-M limit at small μ , and intermediate solutions with the Maugis model are indeed intermediate between DMT-M and JKR. Here, the approximations induced by assuming that no tension is present in the contact region, that the separation is only due to compressive forces, and that the tension is equal to the average value $w/\Delta r$ in the attractive regions, estimated by the first order expansion of displacements, seem to lead to quite conflicting results with respect to the established theories in the entire range of $\mu = 0 - 1$ which we are discussing. Given the DMT-PR theory is then compared with direct simulations using the adhesive potentials, it is not clear how a conflict cannot emerge in numerical simulations, other than perhaps a fortuitous series of error cancellations, or by looking at special range of parameters. There is a high risk however in using this back-of-the-envelope kind of calculation in general conditions.

Obviously, PR geometry of each individual contact probably differs in some cases from that of a sphere, and indeed they suggest they have geometries of contact areas closer to elongated or even "fractal" shapes: whether this can explain the discrepancies in general is not obvious to say. From the typical case of Fig.1, they are looking at nominal area ratios of about 2%, and their bandwidth can be estimated, depending on the system they are studying, to vary between $\alpha = 16$ and 1660. For the low bandwidth cases, the asperity models describe accurately the geometry in contact at these area ratios (Carbone & Bottiglione,

2008), and therefore the system should be very close to an ensemble of Hertzian asperities. It is unclear how therefore their results can be still independent over these wide range of configurations, on Tabor parameter, and on the compression of asperities. Their potentials are truncated in the simulations, but results with full Lennard-Jones potential do not show significant differences, even this factor seems to be ruled out. Interaction effects due to remote forces are possibly causing some different relation between local force and local approach, but this would not change the results.

Notice that for Tabor parameter $\mu = 1$, the x scales in Fig.1 is simply the number of atomic steps of compression, and therefore it is meaningless to look at $\hat{\delta} = \delta / (\mu \Delta r) < 1$. Hence, the adhesive force should be generally *larger* than real. For smaller Tabor parameters $\hat{\delta} = \delta / (10 \Delta r) = 1$ equal to 1 the scale in the plot is a multiple of the number of atomic steps and hence it is realistic to say that the adhesive force will generally be *smaller* than real. Could these two errors balance somehow?

6 Conclusion

We have considered a recent proposal of a very simple extension of the DMT model to general contact problems, including rough contacts, by Pastewka and Robbins. We find, in the known case of sphere, very large possible errors, in part already found in the literature and due to the approximations in DMT theory, which are here exacerbated because of the further simplifications. There is a danger therefore in using these ideas in general.

7 References

- R.S. Bradley, (1932) The cohesive force between solid surfaces and the surface energy of solids. Phil. Mag. 13, 853.
- G.Carboni, & F.Bottiglione, (2008). Asperity contact theories: Do they predict linearity between contact area and load?. Journal of the Mechanics and Physics of Solids, 56(8), 2555-2572.
- B.V. Derjaguin, (1934) Theorie des Anhaftens kleiner Teilchen. Kolloid Zeitschrift 69, 155.
- B.V. Derjaguin, V.M. Muller and Yu.P. Toporov, (1975) Effect of contact deformations on the adhesion of particles. J. Colloid Interface Sci. 53, 314.
- J.A. Greenwood, (2007). On the DMT theory. Tribology Letters, 26(3), 203-211.
- D. Tabor, (1977) Surface forces and surface interactions. J. Colloid Interface Sci. 58, 2.
- D. Maugis and M. Barquins, (1978). Fracture mechanics and the adherence of viscoelastic bodies. J. Phys. D (Appl. Phys.) 11, 1989.

V.M. Muller, V.S. Yuschenko and B.V. Derjaguin, (1980). On the influence of molecular forces on the deformation of an elastic sphere and its sticking to a rigid plane. *J. Colloid Interface Sci.* 77, 91.

V.M. Muller, B.V. Derjaguin and Yu.P. Toporov, (1983) On two methods of calculation of the force of sticking of an elastic sphere to a rigid plane. *Colloids Surf* 7. 251.

M.D. Pashley, (1984). Further consideration of the DMT model for elastic contact. *Colloids Surf* 12, 69.

KL Johnson, K. Kendall, and A. D. Roberts. (1971). Surface energy and the contact of elastic solids. *Proc Royal Soc London A*: 324. 1558.

D Maugis, (2000). Contact, adhesion and rupture of elastic solids (Vol. 130). Springer, New York.

M. D.Pashley, (1984). Further consideration of the DMT model for elastic contact. *Colloids and surfaces*, 12, 69-77.

L. Pastewka, & M.O. Robbins, (2014). Contact between rough surfaces and a criterion for macroscopic adhesion. *Proceedings of the National Academy of Sciences*, 111(9), 3298-3303.